Simulation of Nonlinear Integrable Optics in IOTA Using IMPACT-Z

FAST/IOTA Scientific Program Meeting

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ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION

Outline

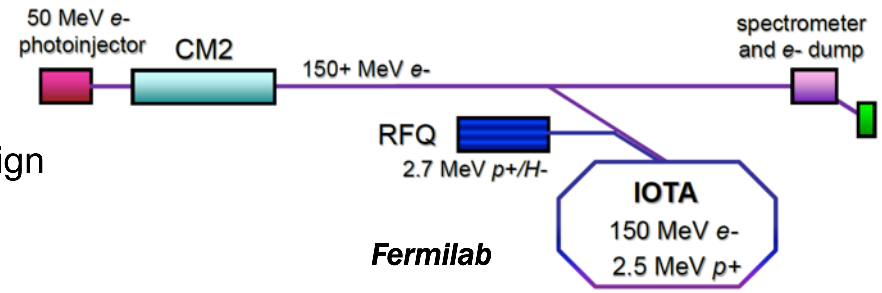
- *Introduction, overview of IMPACT-Z*
- *Modeling nonlinear integrable optics in IOTA*
  - *- first-principles symplectic tracking in the ideal IOTA insert*
  - *- characterization of realistic insert magnetic fields using surface methods (for tracking with fringe fields)*
  - *- understanding the effects of "small-ring" nonlinearities*
- *Near term plans*
- *Conclusions*

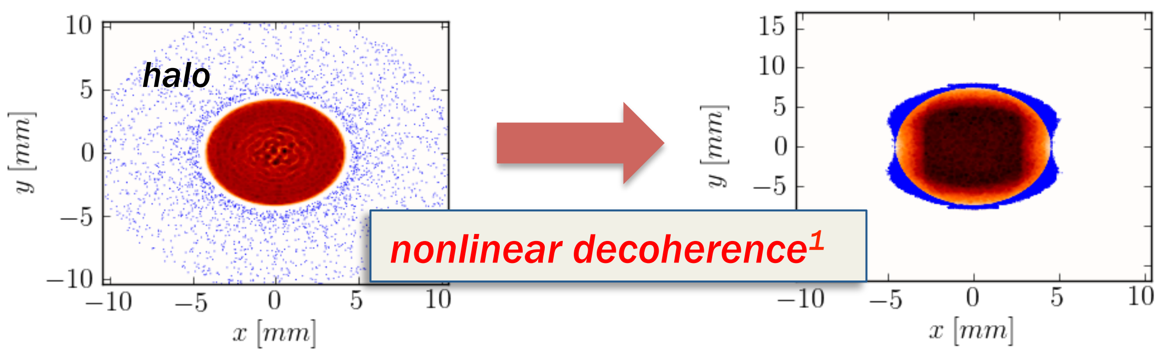
Mitigation of space charge induced beam halo using nonlinear integrable optics in IOTA (with protons)

- **Space charge mitigation: electron lenses/columns, nonlinear integrable lattices**

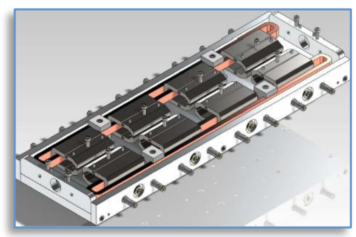
- **Integrable Optics Test Accelerator (IOTA)**

  - Novel accelerator physics: strongly nonlinear design
  - Experimental test bed for SC mitigation schemes
  - Run first with electrons, then low-energy protons





using conventional linear design *using nonlinear integrable design*



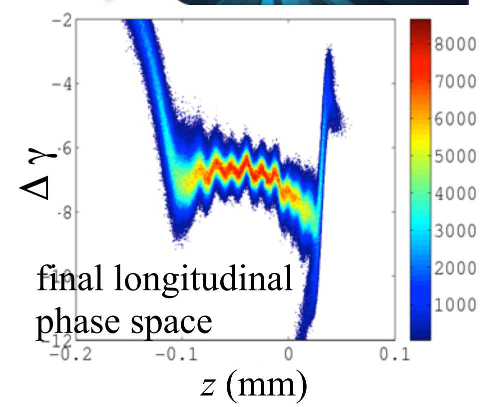
nonlinear magnetic insert

- **Will this work in a real machine? To resolve beam losses at the level needed requires massively parallel long-term tracking with self-consistent space charge.**

[1]S. Webb *et al*, p. 2961, IPAC 2012

Overview of advanced computing/modeling using IMPACT-Z

- **The IMPACT-Z code & physics model**
  - *s-based symplectic particle tracking using maps*
  - *Poisson solvers for 6 distinct boundary conditions*
  - *standard beamline elements, RF and RW wakefields*
  - *field, misalignment, and rotation errors*
  - *multi-turn tracking with simulation restart*
  - *efficient parallelization, access to NERSC*



- **The IMPACT code suite is used by > 40 institutes worldwide**
  - *successfully applied to both electron & proton machines:*
    - *CERN PS2 ring*
    - *LCLS-II linac*
  - *unprecedented resolution: ~2B macroparticles*

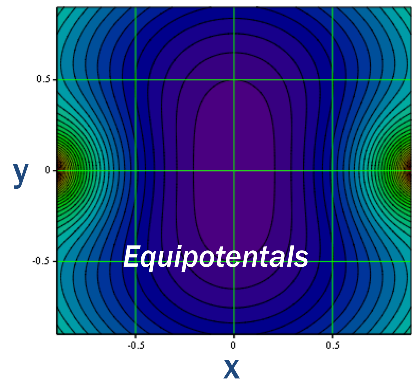
- **First-principles symplectic tracking in the ideal IOTA insert**

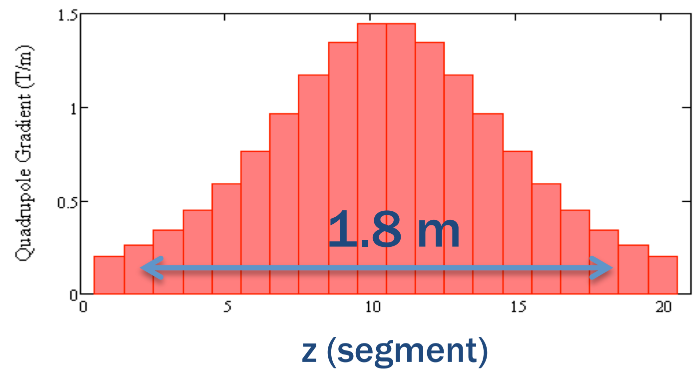
The IOTA magnetic insert was implemented in IMPACT-Z for modeling nonlinear integrable motion.

Nonlinear insert element based on D&N ideal vector potential[1] (compare Synergia)

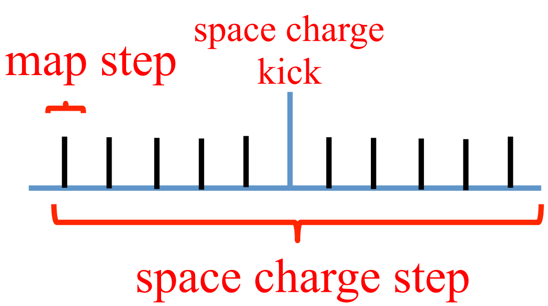
Input arguments: L (m), nSC, nMap, t, c ($m^{1/2}$), μ_0

Novel features allow the user to easily vary the number of segments and SC kicks for numerical convergence studies.





<u>2nd order symplectic integrator</u>



<u>2-level Hamiltonian splitting (Yoshida)</u>

Hamiltonian: $H = H_1 + H_2$

Symplectic map for a step of length τ:

$$\mathcal{M}(\tau) = \mathcal{M}_1\left(\frac{\tau}{2}\right)\mathcal{M}_2(\tau)\mathcal{M}_1\left(\frac{\tau}{2}\right) + O(\tau^3)$$

[1]V. Danilov and S. Nagaitsev, PRSTAB **13**, 084002 (2010)

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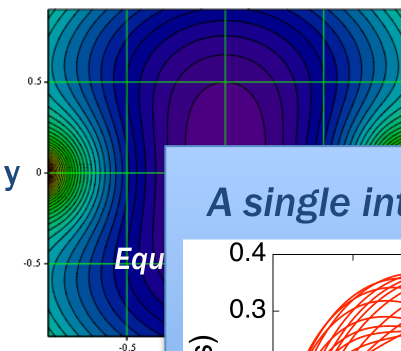
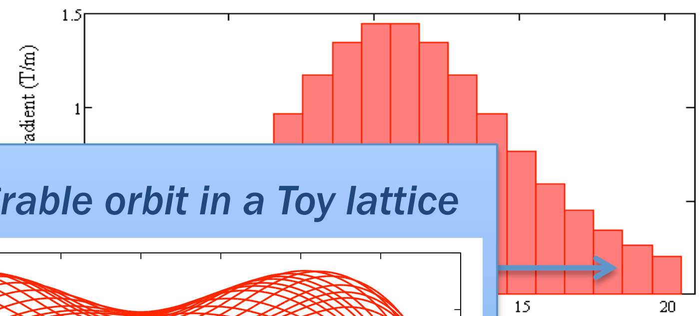
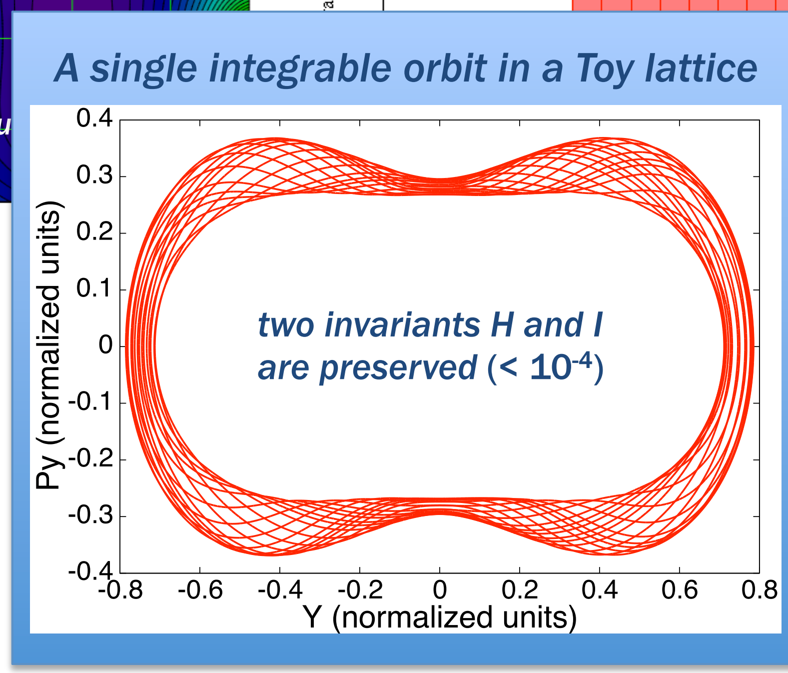
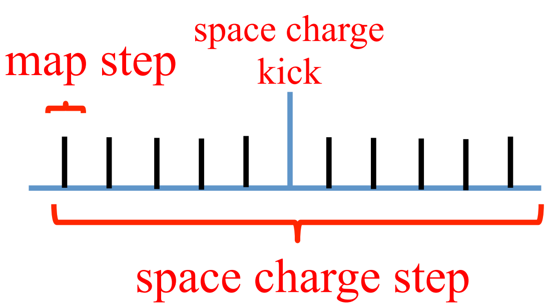






<u>2^{nd} order symplectic integrator</u>



$+ O(\tau^3)$

[1]V. Danilov and S. Nagaitsev, PRSTAB **13**, 084002 (2010)

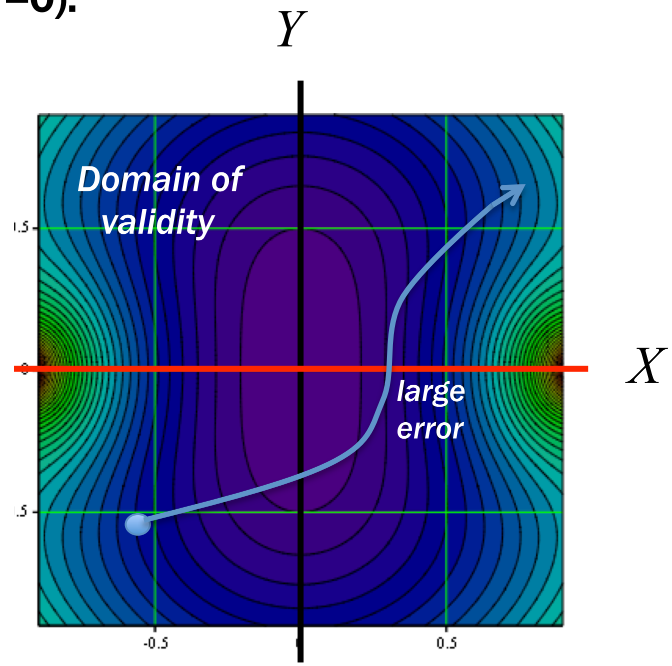
Problem: Original expressions of Danilov and Nagaitsev are not ideal for numerical tracking (complicated, subject to instability).

- **The vector potential takes a complicated form that relies on a variable transformation in the plane (*X,Y*) that is poorly behaved in the midplane (*Y*=0).**

$$\xi = \frac{\sqrt{(x+f)^2+y^2}+\sqrt{(x-f)^2+y^2}}{2f},$$

$$\eta = \frac{\sqrt{(x+f)^2+y^2}-\sqrt{(x-f)^2+y^2}}{2f}$$

vanishing Jacobian →



- **Derivatives of the vector potential are built from expressions with vanishing denominators in the midplane.**

$$(\partial_x, \partial_y) \rightarrow (\partial_\xi, \partial_\eta) \quad \text{not invertible}$$

- Particles that cross the midplane repeatedly → runaway coordinates and momenta.

- This can be avoided using Taylor series in *Y*, with a resulting loss in numerical accuracy.

New first-principles theory of 2D nonlinear integrable potentials: concise, simple, and avoids a numerical instability.

Integrability requires that we search for a 2D magnetic vector potential A_s satisfying:

2D Laplace Eq. (in X,Y) ***Bertrand-Darboux Eq.***

$$(\partial_x^2+\partial_y^2)\mathcal{A}_s=0\,,\qquad xy(\partial_x^2-\partial_y^2)\mathcal{A}_s+(y^2-x^2+1)\partial_x\partial_y\mathcal{A}_s+3y\partial_x\mathcal{A}_s-3x\partial_y\mathcal{A}_s=0$$

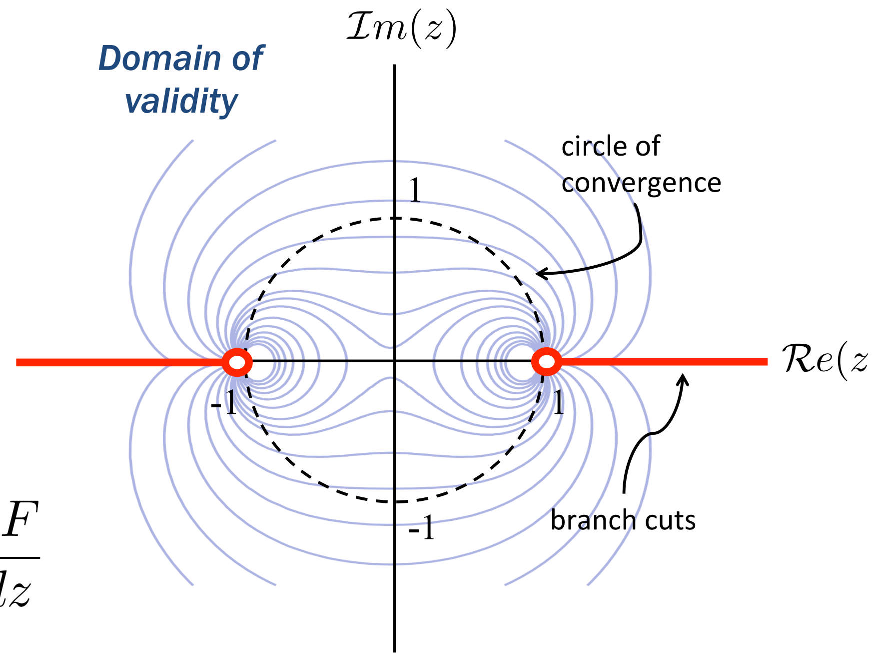
$$z=x+iy \qquad F=\mathcal{A}_s+i\psi$$

Complex representation as a single ODE:

$$(z^2-1)\frac{d^2F}{dz^2}+3z\frac{dF}{dz}+2\tilde{t}=0$$

Simple solution:

$$F(z)=\left(\frac{\tilde{t}z}{\sqrt{1-z^2}}\right)\arcsin(z)\,,\quad p^*=\sigma\frac{dF}{dz}$$



C. E. Mitchell, "Complex Representation of Potentials and Fields for the Nonlinear Magnetic Insert of the Integrable Optics Test Accelerator," LBNL-1007217 (2017), *to be submitted* Phys. Rev. ST Accel. Beams

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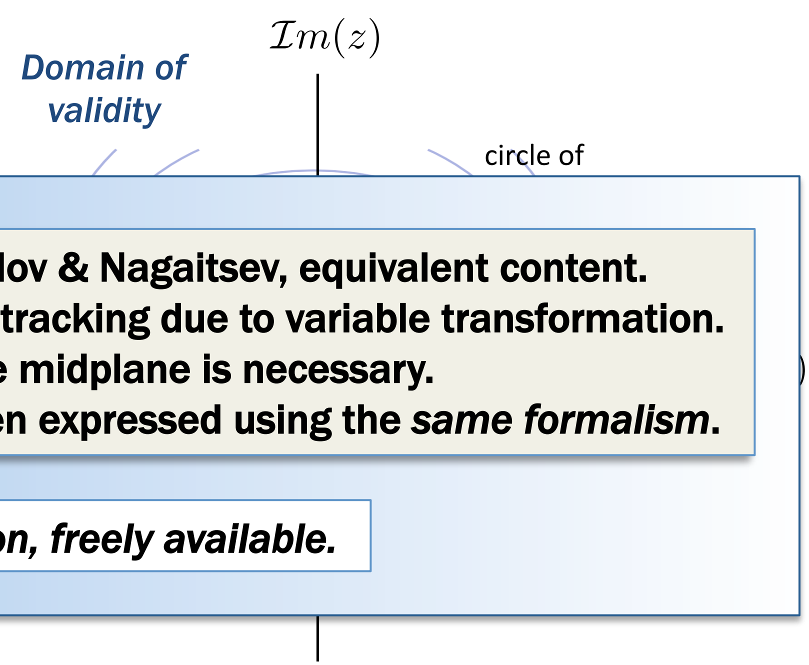
$$z = x + iy \qquad F = \mathcal{A}_s + i\psi$$



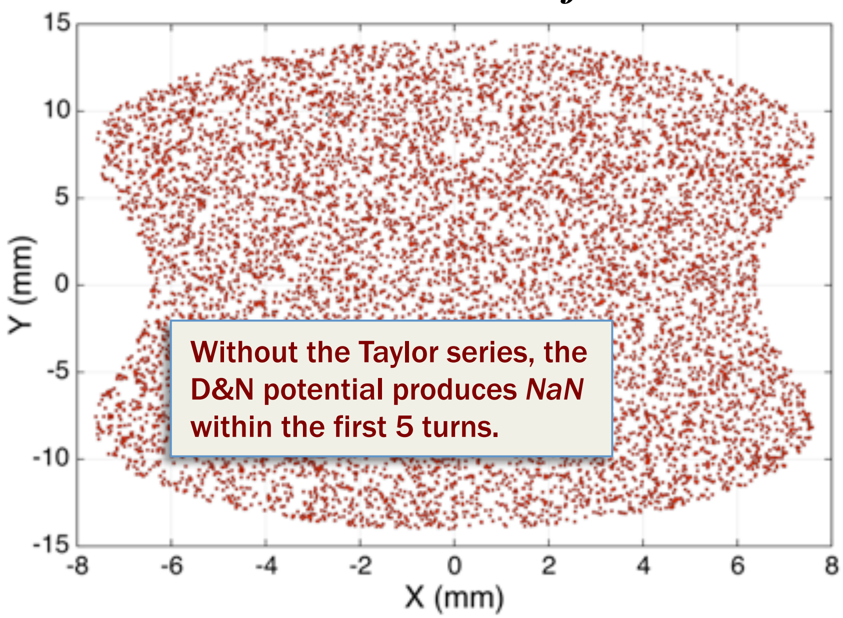
- *Much simpler* than the original expressions of Danilov & Nagaitsev, equivalent content.
- Avoids small denominators in the midplane during tracking due to variable transformation.
- No Taylor expansion of the vector potential near the midplane is necessary.
- The invariants of motion (key diagnostics) have been expressed using the *same formalism*.

Code distributed to IOTA collaboration, freely available.

C. E. Mitchell, "Complex Representation of Potentials and Fields for the Nonlinear Magnetic Insert of the Integrable Optics Test Accelerator," LBNL-1007217 (2017), *to be submitted* Phys. Rev. ST Accel. Beams

Tracking Implementation Using a Complex Potential: Matched KV Beam Benchmark in the Toy Lattice (100 Turns)

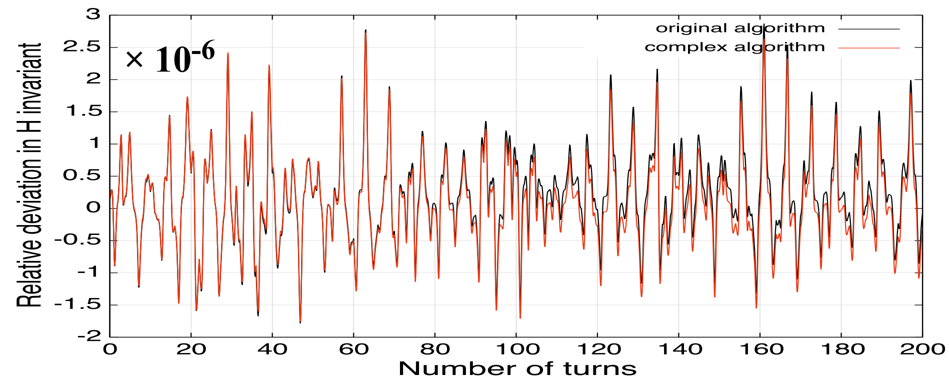
Final beam distribution after 100 turns



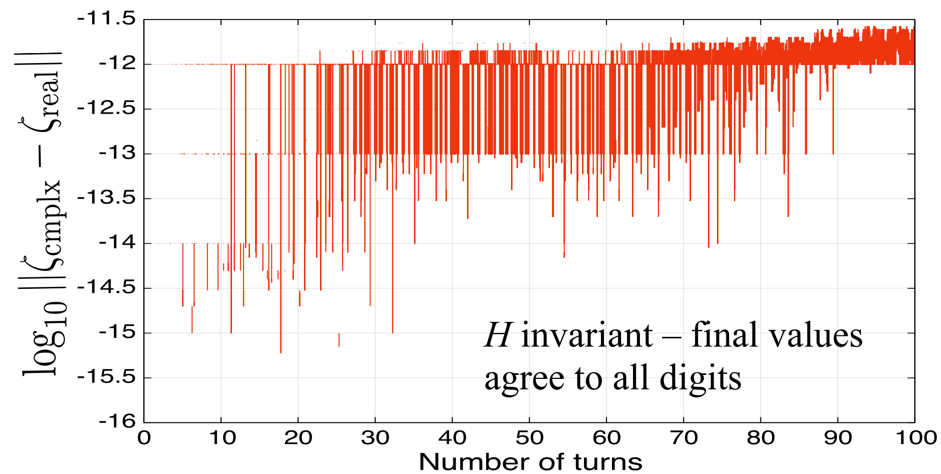
● final particle distribution obtained using original algorithm based on real-valued potential from D&N (*with* Taylor series)

● final particle distribution obtained using algorithm based on complex potential

First moment of the H invariant



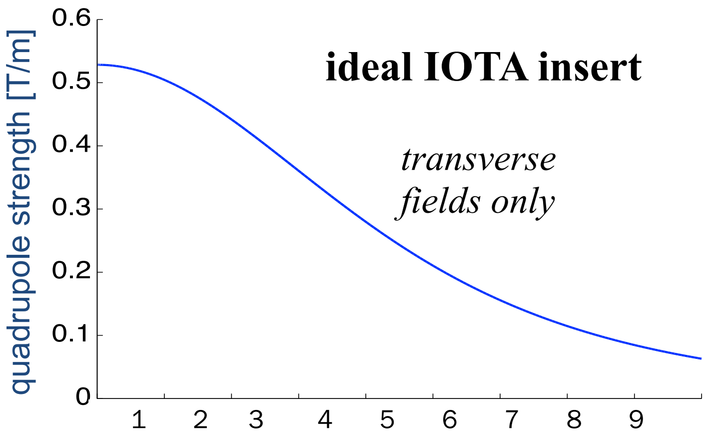
Numerical difference in a single orbit

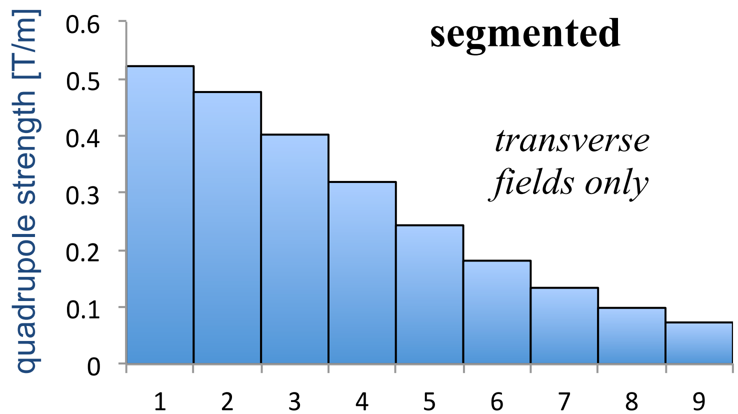


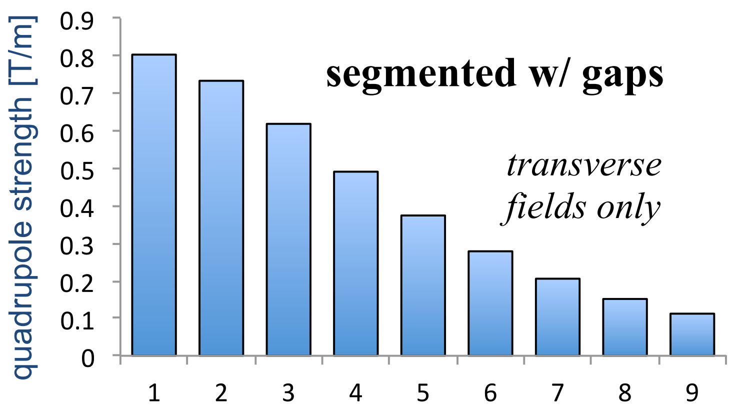
- Characterization of realistic insert magnetic fields using surface methods (for tracking with fringe fields)

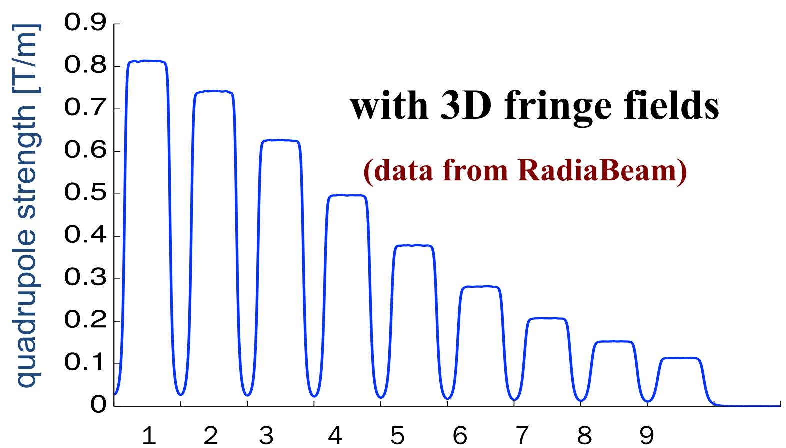
Problem: The idealized model of the IOTA insert is non-Maxwellian, and neglects fringe field/segment effects.

- Consider the following sequence of approximations (insert shown from midpoint to exit):









What is needed: a concise, smooth representation of the insert vector potential based on 3D magnetic field data.

- For extracting symplectic maps *or* using a symplectic integrator, one begins with a Hamiltonian of the form (straight element, s as the independent variable):

$$H(x,p_x,y,p_y,t,p_t;s) = -\sqrt{\frac{p_t^2}{c^2} - m^2c^2 - (p_x - qA_x)^2 - (p_y - qA_y)^2} - qA_s$$

- Typically, it is necessary or beneficial to perform a Taylor series about the design trajectory through the beamline element, which will require a Taylor series in A_x, A_y, A_s in the transverse variables x, y.

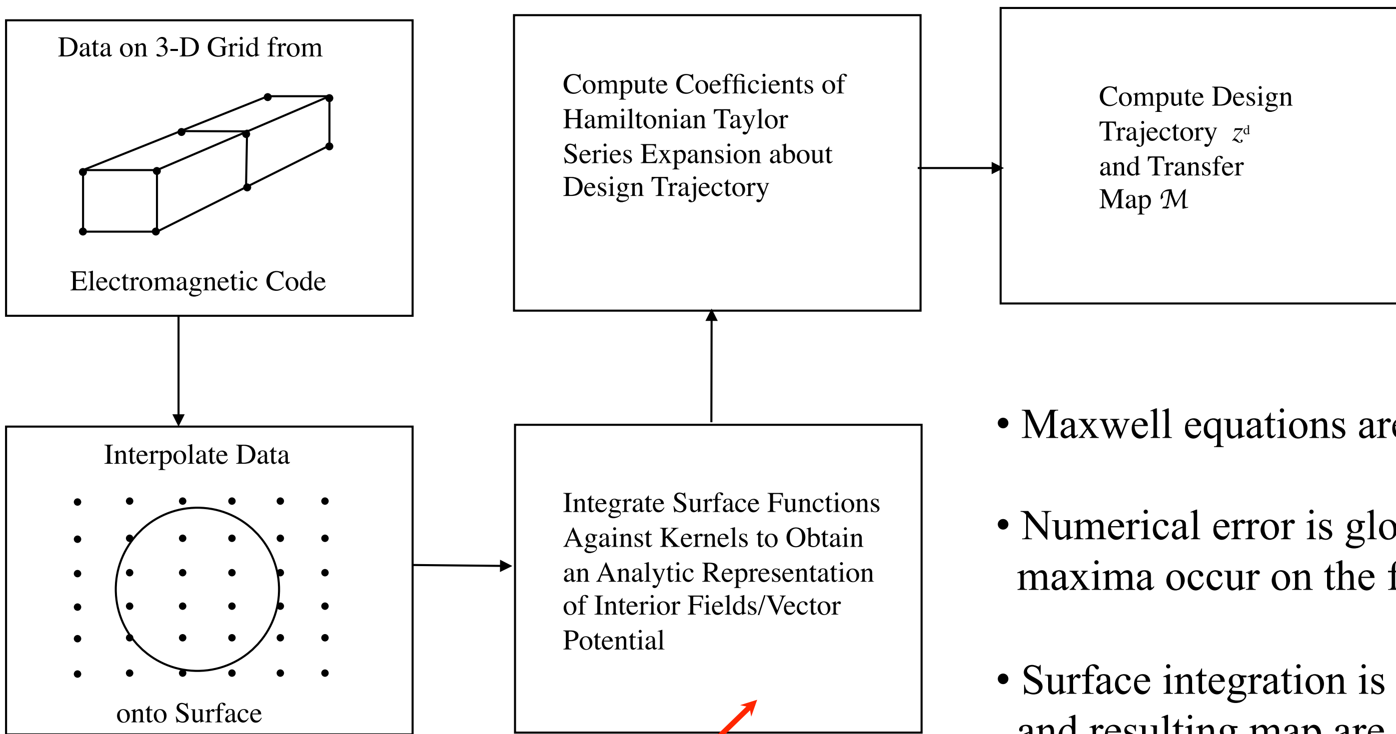
➢ **How do we extract a vector potential A from a magnetic field B on a grid?**

➢ **How do we reliably extract the Taylor coefficients of A (or its derivatives)?**

Limited by numerical noise in the data!

Solution: Use surface methods to extract a vector potential and transfer map from 3D magnetic field data.

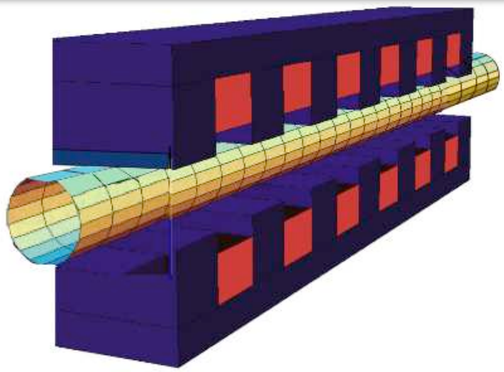
Surface methods provide a well-established technique for extracting high-order derivative information in the presence of noise by exploiting the structure of Maxwell's equations.



Use Green's function for special domains (cylinder, box)

- Maxwell equations are exactly satisfied.
- Numerical error is globally controlled – maxima occur on the fitting boundary.
- Surface integration is *smoothing* – derivatives and resulting map are robust and insensitive to numerical errors.

Generalized gradients provide a robust, complete description of the 3D vector potential using surface data.



Reference trajectory is a straight line or nearly a straight line along the axis. Normal component of ***B*** on a cylinder is used.

Expansion of $\psi(x,y,s)$ as a power series in x and y →

Power series for the vector potential **A** in the Coulomb gauge[1]:

$$A_{\left\{\begin{smallmatrix}x\\ y\end{smallmatrix}\right\}} = \sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\frac{(-1)^l m!}{2^{2l+1}\, l!(l+m+1)!}(x^2+y^2)^l\left[\mathrm{Re}(x+iy)^{m+1}C^{[2l+1]}_{m,\left\{\begin{smallmatrix}s\\ c\end{smallmatrix}\right\}}(s)\mp\mathrm{Im}(x+iy)^m C^{[2l+1]}_{m,\left\{\begin{smallmatrix}c\\ s\end{smallmatrix}\right\}}(s)\right]$$

$$A_z = \sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\frac{(-1)^l m!}{2^{2l}\, l!(l+m)!}(x^2+y^2)^l\left[-\mathrm{Re}(x+iy)^m C^{[2l]}_{m,s}(s)+\mathrm{Im}(x+iy)^m C^{[2l]}_{m,c}(s)\right]$$

where the *generalized gradients* are given by[2]:

Fourier coefficients of normal ***B*** field on the surface.

$$C^{[n]}_{m,\alpha}(s) = \frac{i^n}{2^m m!}\int_{-\infty}^{\infty}\frac{k^{n+m-1}}{I'_m(kR)}\tilde{B}^{\alpha}_{\rho}(R,m,k)e^{iks}dk$$

[1]C. Mitchell and A. Dragt, Phys. Rev. ST Accel. Beams **13**, 064001 (2010).
[2]M. Venturini and A. Dragt, Nucl. Instrum. and Meth. Phys. Res. A **427**, 387 (1999).

The generalized gradients for the ideal IOTA insert can be determined analytically (for benchmarking).

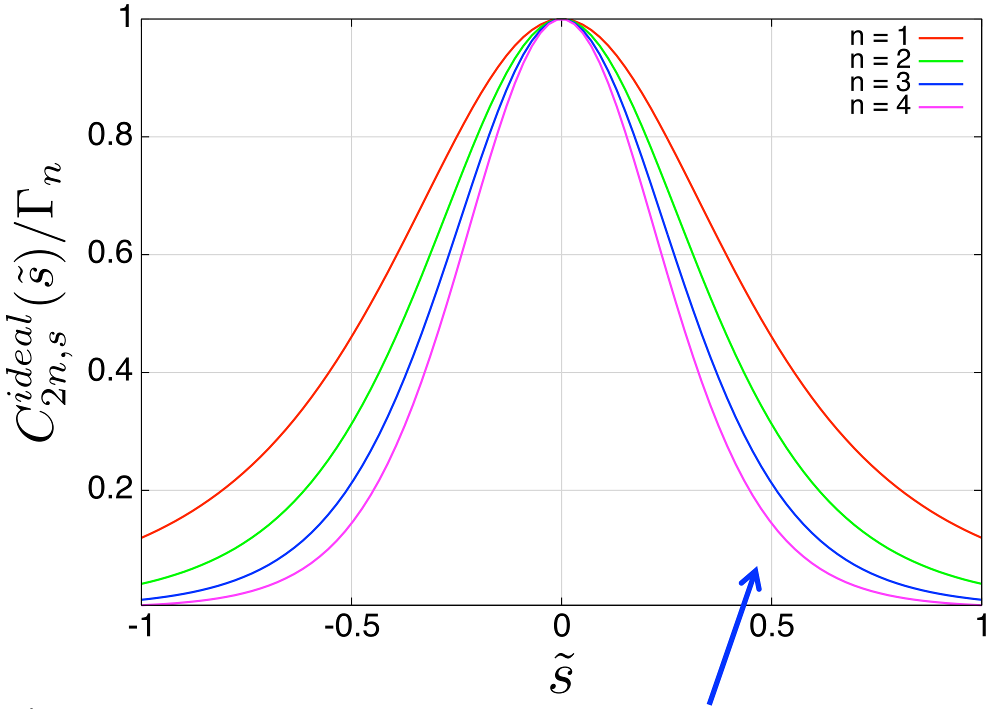
Generalized gradients m=2 (quadrupole) through m=8 are shown for the nominal phase advance of $\mu_0 = 0.3$.

Each quantity is normalized by its value at the magnet midpoint (s=0).

$$C_{2n,s}^{ideal}(\tilde{s}) = \frac{\Gamma_n}{\{1+\tilde{s}^2\tan^2(\pi\mu_0)\}^{n+1}}$$

$$\tilde{s} = 2s/L$$

Generalized Gradients of the Ideal IOTA Insert



size of derivatives are controlled by phase advance

Values at the magnet midpoint are given by:

$$\Gamma_n = -\tau\left(\frac{B\rho}{c^{4n}}\right)\frac{2^{2n-1}n!(n-1)!}{(2n)!}\left(\frac{c^2}{\beta^*}\right)^{n+1}, \quad \beta^* = \frac{L}{2}\cot(\pi\mu_0)$$

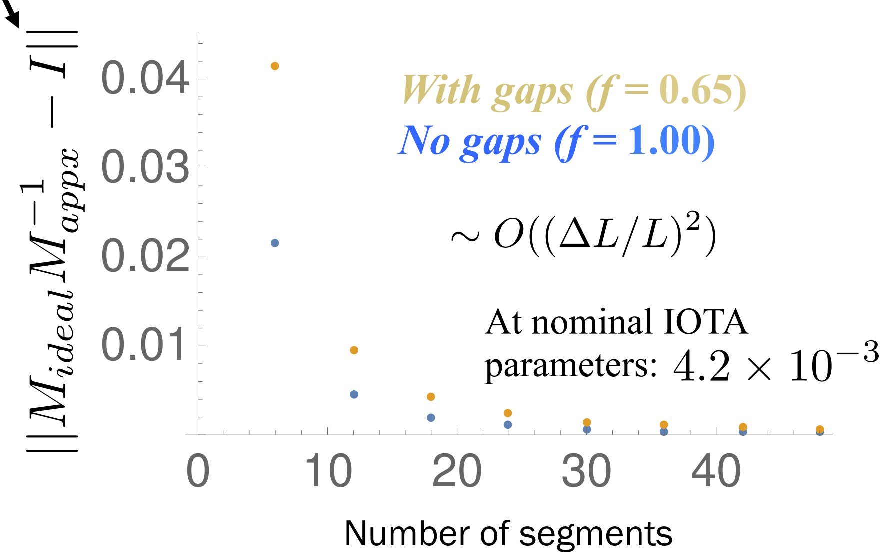
Fed into the Hamiltonian to extract the linear map + Lie generators via map equations.

The linear map was determined exactly and used to study the effects of introducing segments and gaps.

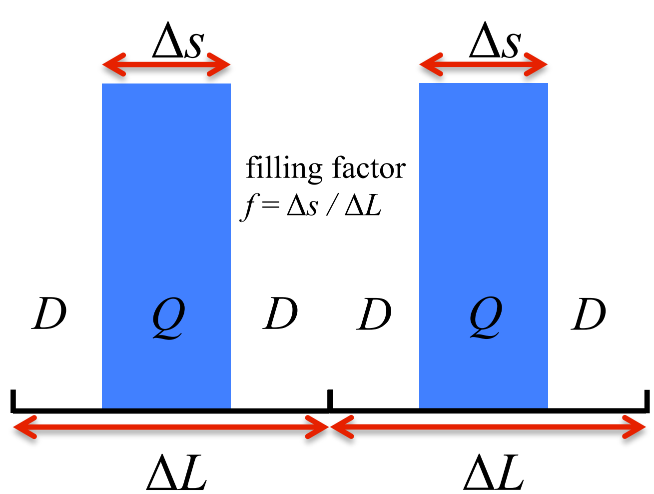
- Example: Quadratic convergence to the ideal linear map as the number of segments is increased, while the filling factor is held fixed. (τ =0.45, μ_0=0.3, L=1.8 m)

matrix spectral norm

Convergence with number of segments

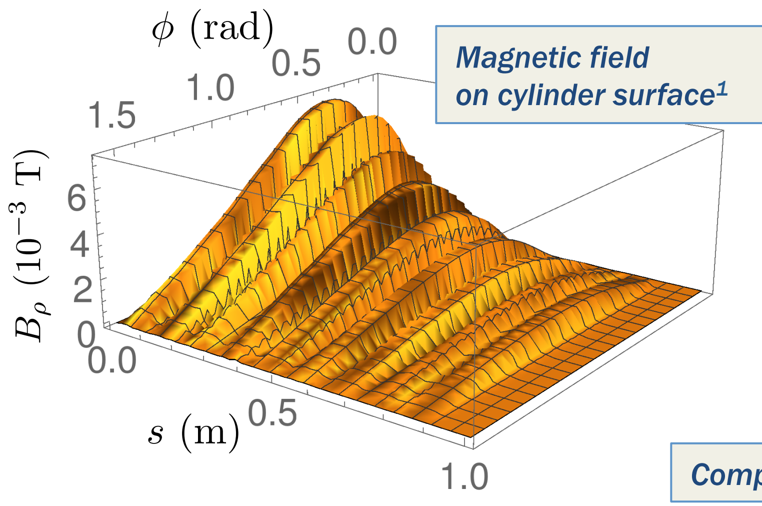


Model for insert segments and gaps



- Work is underway to investigate the nonlinear generators for the factorized Lie map of the IOTA insert, using tools available in MaryLie/IMPACT.

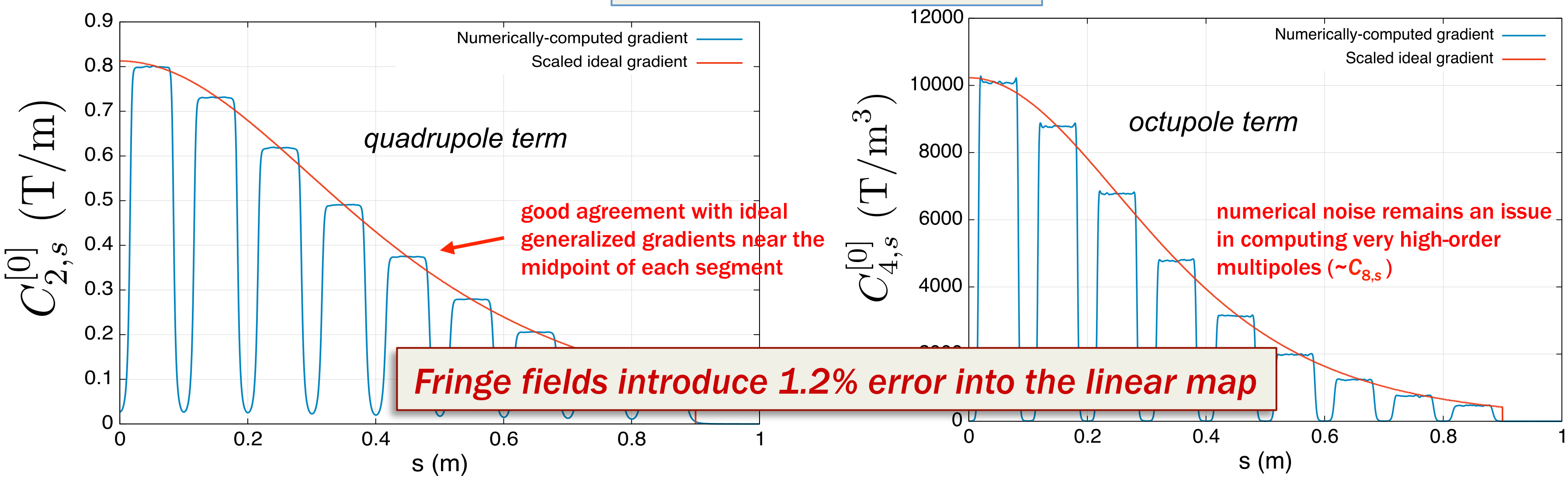
Generalized gradients were extracted from RadiaBeam 3D magnetic field data using surface methods.



Magnetic field on cylinder surface[1]

Parameter	Symbol	Value	Unit
Strength parameter	τ	0.45	-
Transverse scale factor	c	0.009	$m^{1/2}$
Phase advance across NLI	μ_0	0.3	-
Length of NLI	L	1.8	m
Beta at NLI midpoint	β^*	0.6538	m
Segment length	Δs	6.5	cm
Magnetic rigidity (150 MeV e^-)	$B\rho$	0.502	T-m

Computed generalized gradients



Fringe fields introduce 1.2% error into the linear map

[1]Data provided by F. O'Shea (RadiaBeam). See eg, F. O'Shea *et al*, PAC2013.

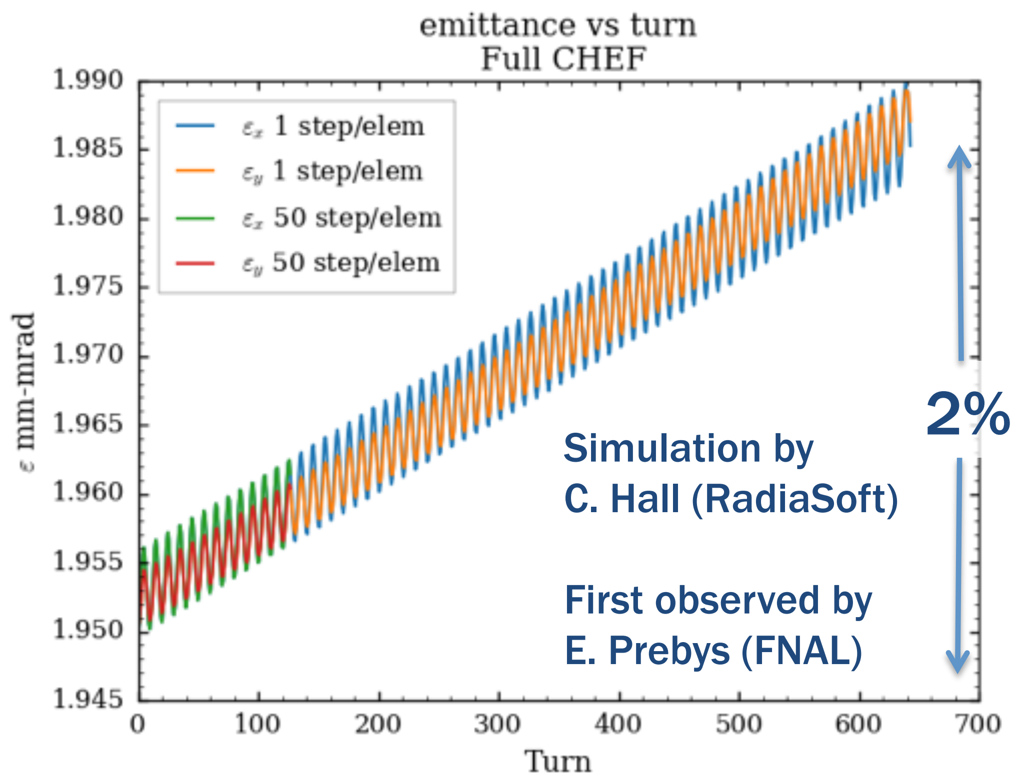
- **Understanding the effects of “small-ring” nonlinearities**

Problem: Unexpected linear emittance growth observed in the IOTA lattice (insert *off*, no SC) using Synergia.

Similar emittance growth not observed in previous tracking studies using the code PTC.

Problem traced back to a *non-symplectic* 2nd-order thin lens fringe field kick applied at dipole entrance/exit in Synergia (under repair).

Suggests the importance of *accurate fringe field models*, and the possible importance of fringe field and other "small ring" nonlinearities to IOTA performance.

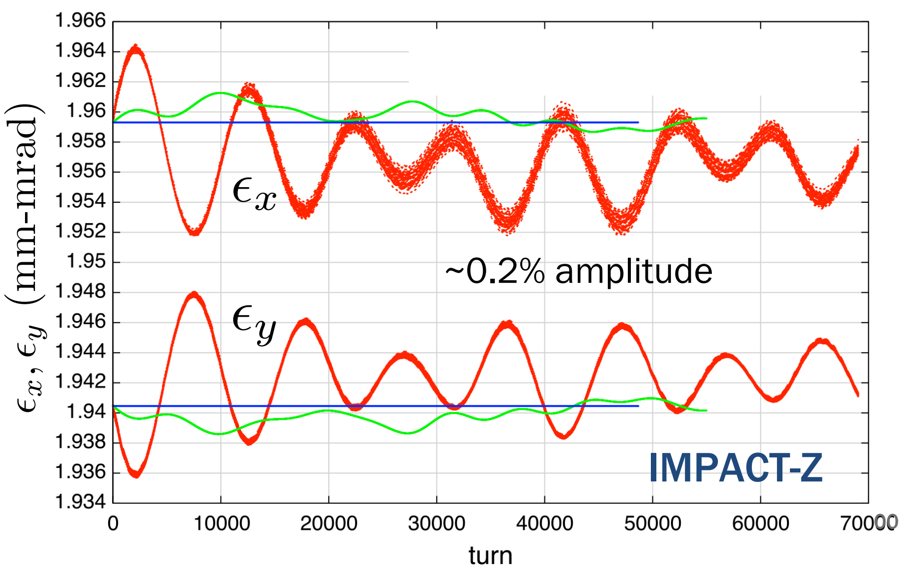


In Synergia studies of IOTA with space charge, the arc external to the insert is typically linearized in order to make theoretical progress in understanding the interplay between SC and integrability.

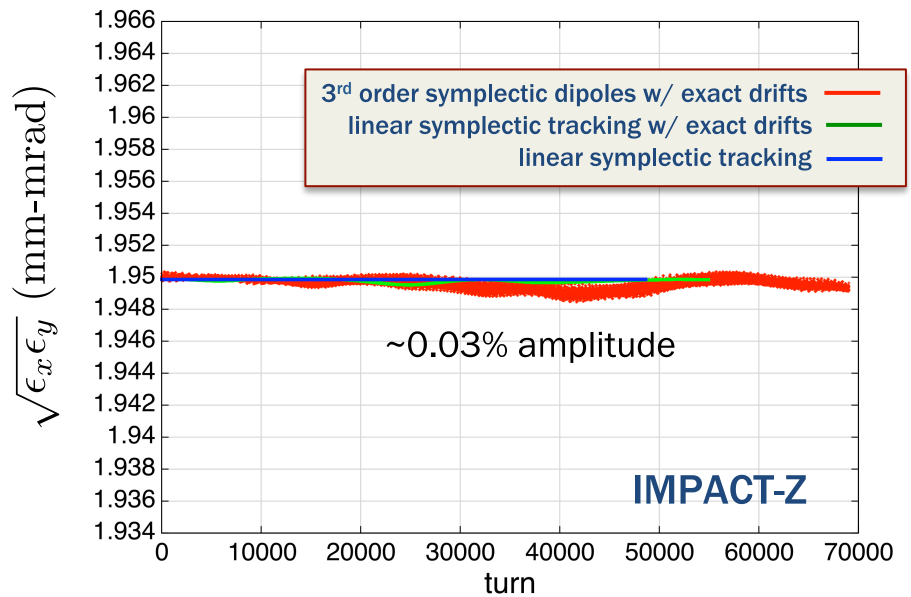
Significant emittance growth is not observed over ~100K turns in IMPACT-Z (insert *off*, no SC).

- Tracking performed using both IMPACT-Z and ML/I. Initial emittance (rms): *1.95 mm-mrad*.
- Both codes use a 3rd-order symplectic dipole model with 3rd-order hard-edge fringe fields.

Horizontal and vertical emittances



Geometric mean of emittances



Long-term tracking studies reveal that kinematic and dipole nonlinearities lead to acceptable bounded oscillations in both *X*, *Y* emittance with an amplitude of ~0.2%.

A complete, realistic treatment of dipole fringe fields requires the use of surface methods.

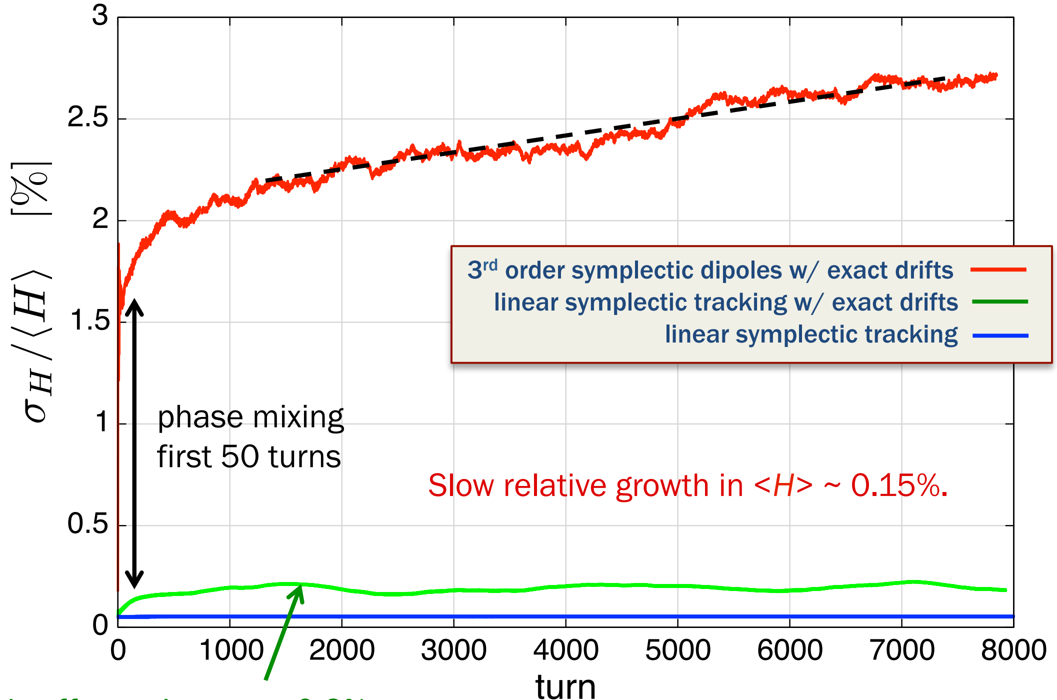
In the IOTA lattice (insert *on*, no SC), 2nd/3rd-order dipole effects lead to diffusion of the two invariants.

<u>IOTA Lattice (2.5 MeV p)</u>
2 nonlinear inserts *ON*
L=1.8 m, t=0.45,
c = 0.009 $m^{1/2}$, μ_0=0.3
Matched nonlinear KV beam
ε_0 = 3.9 mm-mrad, σ_δ = 0

Rapid mixing over the first 2-3 turns, followed by slow diffusion.

- constant if *H* invariant is preserved
- zero for a "nonlinear KV" distribution

Diffusion of the H invariant (IMPACT-Z)



Kinematic effects plateau at 0.2%.

The corresponding value of $\sigma_I/\langle I\rangle$ (for the second invariant) grows by 1% over 8000 turns.

Expected to be less problematic for a large ring such as the proposed Rapid Cycling Synchrotron.

Scaling of kinematic and dipole nonlinear effects with initial beam emittance (σ_H evaluated at turn 2,000)

Larger-emittance beams sample stronger non-ideal nonlinear effects.

Clear scaling trend for the size of dipole-induced diffusion of the H invariant.

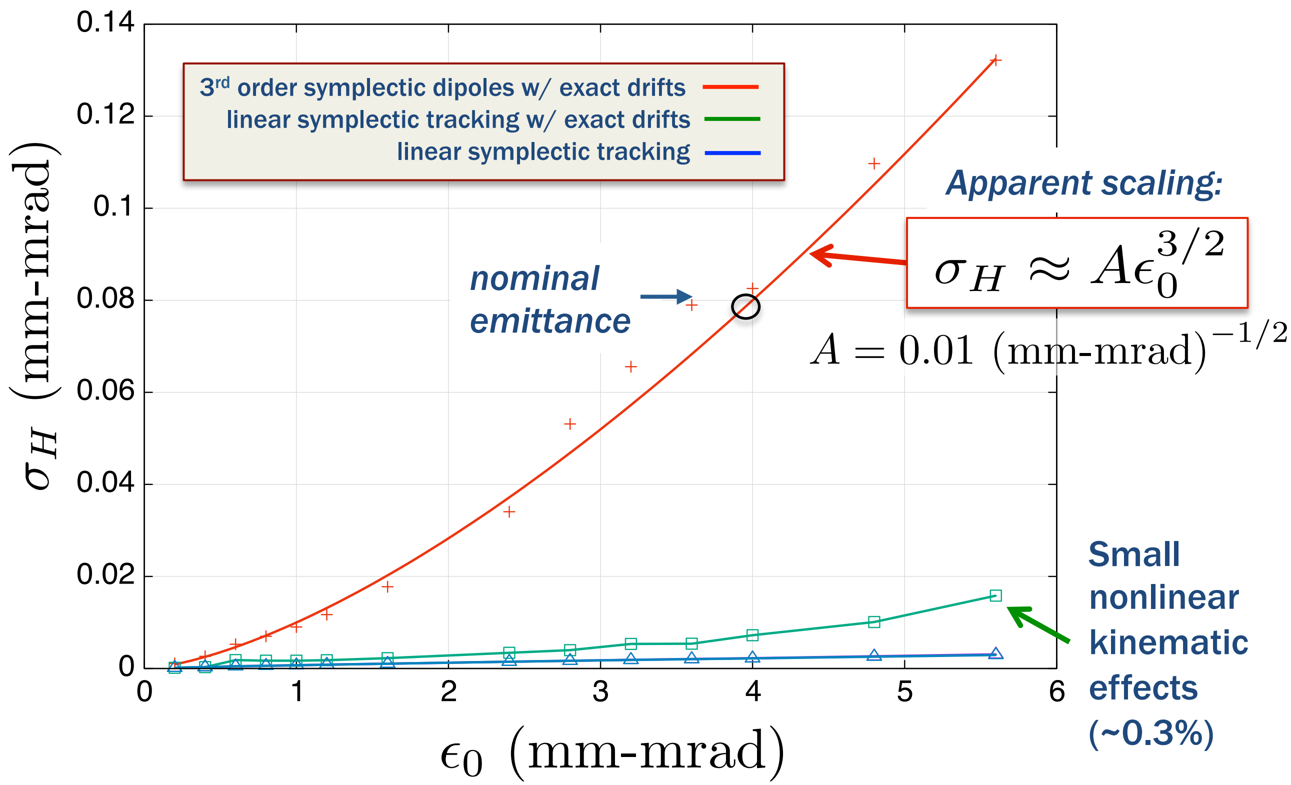
Scaling trend continues up to ε_0 ~ 8 mm-mrad.

Parameters are the same as those on the previous slide.

Note $\sigma_H/\langle H\rangle \sim \sqrt{\epsilon_0}$.

To ensure $\sigma_H/\langle H\rangle < 2\%$ **requires** ε_0 **< 4 mm-mrad.**

Growth in σ_H after 2K turns (IMPACT-Z)



Near-Term Plans

Over the next several months:

- **Additional studies using the generalized gradient series for the nonlinear insert to investigate fringe field effects on long-term evolution of the two invariants.**

- **Benchmarking of Impact-Z simulations of the full nonlinear IOTA lattice with space charge (insert *on*) against Synergia at moderate resolution before scaling up simulation size.**

- **Collaboration with Fermilab, RadiaSoft to study the limits of existing space charge algorithms for the challenging case of intense long, bunched beams with space charge.**

- **Implementation of the location-dependent physical aperture for the IOTA lattice into the existing Impact-Z model to enable beam loss prediction.**

Conclusions

- New numerical tools are needed for studying high-resolution halo formation, beam losses, and errors in the presence of nonlinear integrable optics, while avoiding artifacts due to numerical noise. Such studies may be critical to successful proton operation in IOTA.
- Cross-checks among several codes (Synergia, Impact-Z, WARP…) are critical to gain confidence in simulations of nonlinear integrable optics with space charge.
- Impact-Z contains scalable and robust Poisson solvers that are ideal for high-resolution, long-term studies of collective space charge instabilities, and additional capabilities have now been implemented that will aid in high-fidelity simulation of IOTA.
- Successful benchmarks have been performed of the nonlinear insert, matched beam generation, linear lattice optics, and space charge capabilities, and studies have begun to reveal interesting physics.

- **Backup slides**

Milestones for Task Area 1: toward high-fidelity simulation of the IOTA lattice (reported Dec. 21, 2016)

- ✓ Implementation of the IOTA nonlinear magnetic insert in IMPACT-Z.
- ✓ Implementation of new IOTA-specific diagnostic output in IMPACT-Z, for characterizing statistics of the two invariants and normalized phase space coordinates.
- ✓ Successful benchmarking of the IOTA nonlinear insert without space charge.
- ✓ Development of a new diagnostic tool for characterizing beam mismatch to the nonlinear lattice.
- ✓ Improvements in the Python MAD-X – Impact-Z lattice parser, to easily generate IMPACT-Z input files from IOTA lattice files (provided in MAD-X).
- ✓ Successful benchmarking of the linear IOTA lattice with and without space charge (against Synergia+WARP).

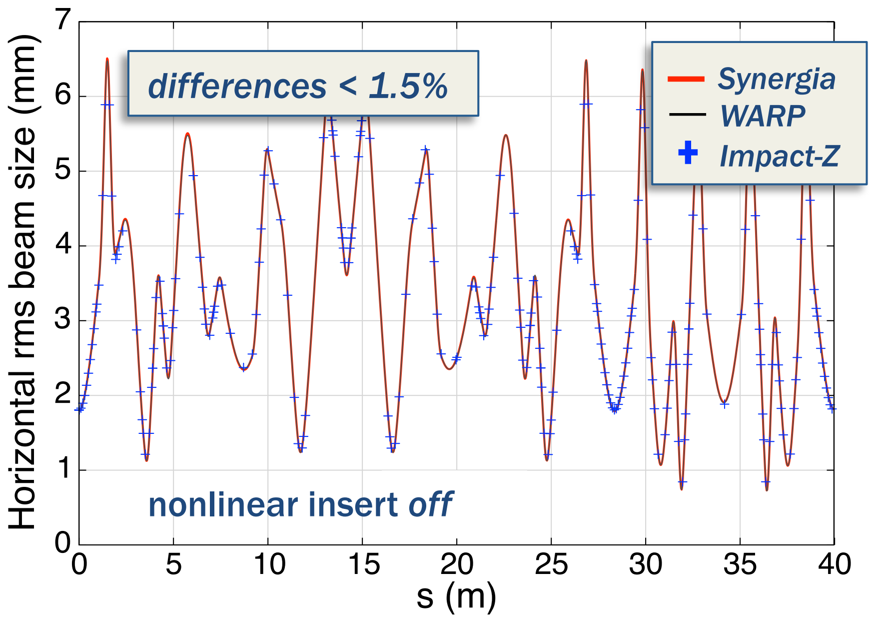
Milestones for Task Area 1: toward high-fidelity simulation of the IOTA lattice (since Dec. 21, 2016)

- ✓ New analytical treatment of the Bertrand-Darboux equation for integrable potentials.
- ✓ Development and distribution of an improved tracking model through the ideal IOTA nonlinear insert using complex potentials (avoids runaway particles, numerical artifacts).
- ✓ Use of surface methods/generalized gradients to characterize the physical IOTA nonlinear insert magnetic field (RadiaBeam) to allow realistic tracking with fringe fields.
- ✓ Investigation of long-term emittance growth (100K turns) due to nonlinear effects in the IOTA lattice without the insert present – fringe fields and nonlinear kinematic effects.
- ✓ Benchmarking between IMPACT-Z and ML/I (with R. Ryne), with the goal of map analysis.
- ✓ Improvements in the IMPACT-Z quadrupole model, relevant for *p* operation (low energy).

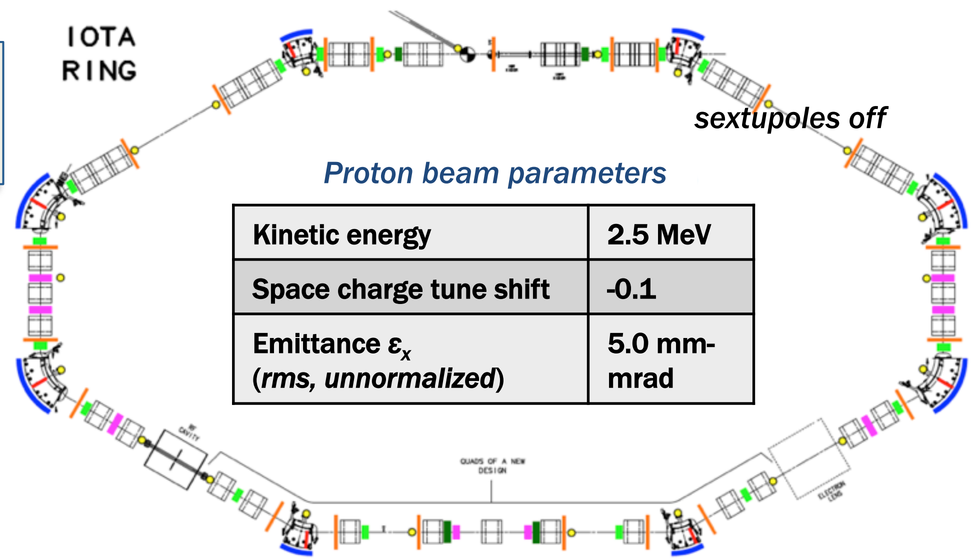
Beam dynamics in IOTA provides a challenging test-bed for numerical space charge benchmarking.

- Good agreement between Impact-Z, WARP, and Synergia over 50 turns.
- Impact-Z is *critical* to provide cross-checks of Synergia, and scales efficiently to large number of particles and grid points. (Synergia simulation by C. Hall, WARP simulation by R. Kishek.)

Impact-Z simulation uses 1M particles, 32x32x1025 grid, longitudinally periodic BC.



Horizontal RMS Envelope – Turn 50



Proton beam parameters

Kinetic energy	2.5 MeV
Space charge tune shift	-0.1
Emittance ε_x (*rms, unnormalized*)	5.0 mm-mrad

- $\beta_x = \beta_y$, $D = 0$ across the nonlinear drift space
- $n\pi$ phase advance from nonlinear drift space exit to nonlinear drift space entrance

Symplectic integrator options for the ideal IOTA magnetic insert in IMPACT-Z

$$\boxed{H = H_D + H_{NLL}}$$

Step of size τ: $\mathcal{M}_H(\tau) \approx \mathcal{M}_D\left(\frac{\tau}{2}\right)\mathcal{M}_{NLL}(\tau)\mathcal{M}_D\left(\frac{\tau}{2}\right)$

1) Exact Hamiltonian splitting:

$$H = -\sqrt{1 - \frac{2P_t}{\beta_0} + P_t^2 - P_x^2 - P_y^2} - \frac{P_t}{\beta_0} - \mathcal{A}_s(X,Y) \longrightarrow H_{NLL}$$

2) Paraxial drift splitting:

$$H = \frac{1}{2}\Delta\left(P_x^2 + P_y^2\right) - \left(\frac{1}{\Delta} + \frac{P_t}{\beta_0}\right) - \mathcal{A}_s(X,Y)$$

$$\Delta = \frac{1}{\sqrt{1 - 2P_t/\beta_0 + P_t^2}} = \frac{1}{1+\delta}$$

3) Linearized drift splitting:

$$H = \frac{1}{2}\left(P_x^2 + P_y^2\right) + \frac{P_t^2}{2\beta_0^2\gamma_0^2} - \mathcal{A}_s(X,Y)$$

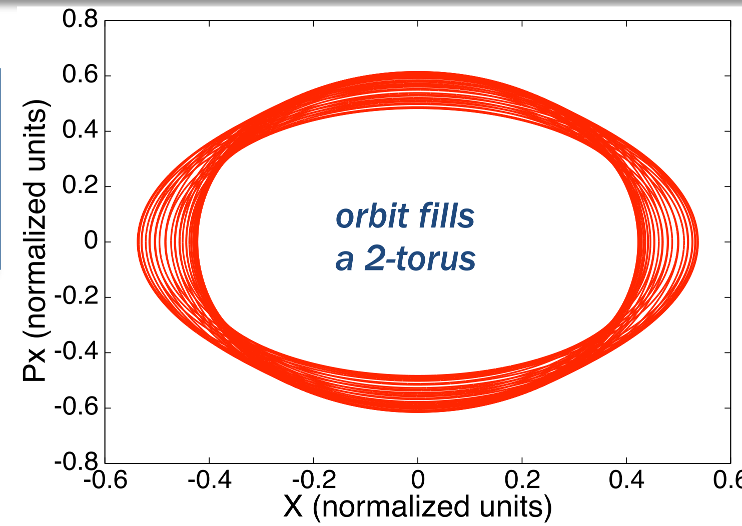
In the special case when δ = 0, note that 2) and 3) are equivalent.

Single-particle tracking using the nonlinear insert: integrable motion in the Toy benchmark lattice

Insert parameters

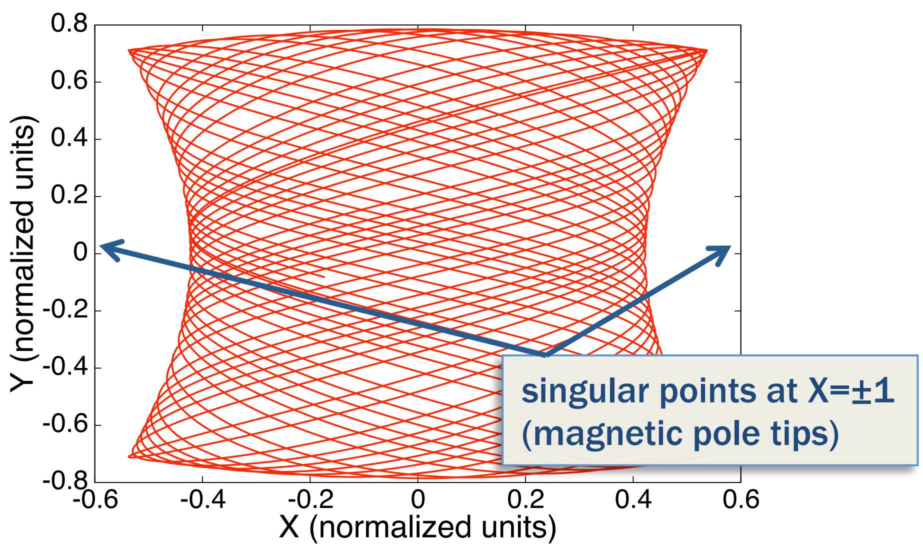
$t = 0.45$
$\mu_0 = 0.3$
$L = 2.0$ m
$c = 0.01\ \mathrm{m}^{1/2}$

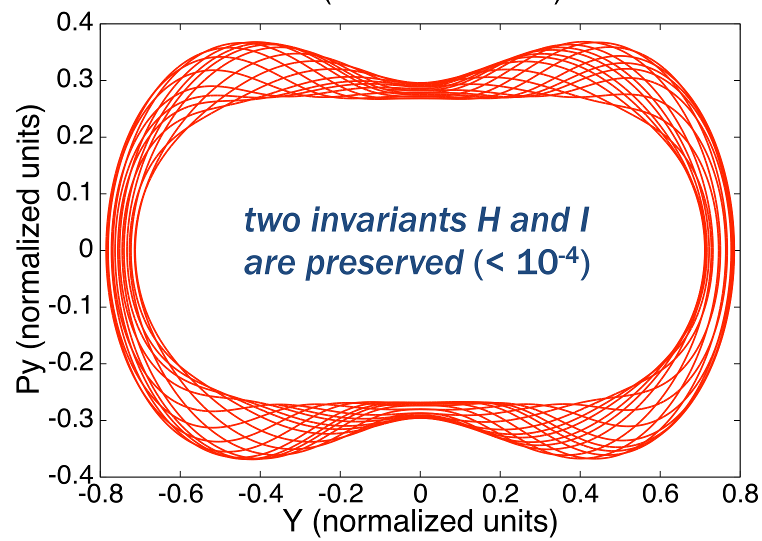
- lattice consists of nonlinear insert + a linear focusing lens
- a single orbit is shown over 100 turns



Initial conditions (normalized)

$(x,p_x,y,p_y) = (-0.173,-0.558,-0.082,0.284)$





Nonlinear matched beam generation has been successfully coupled with IMPACT-Z simulation.

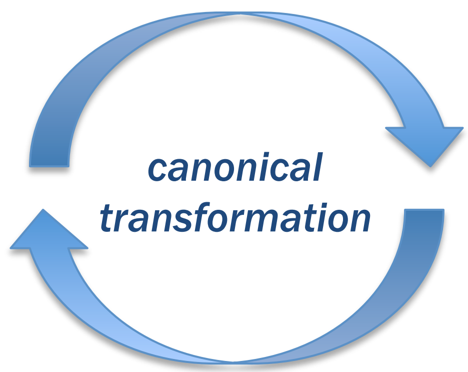
Matching to the nonlinear lattice is nontrivial and may be critical to beam performance.

normalized phase space variables (x_N, x'_N, y_N, y'_N)

"nonlinear KV distribution" [1]

$$f \sim \delta(H - \epsilon_0)$$

- Hamiltonian is *s*-independent
- distribution function is stationary



physical phase space variables (x, x', y, y')

- Hamiltonian is *s*-dependent
- distribution varies periodically in *s*
- parameter ε_0 plays the role of emittance

- **Shared Python scripts developed by RadiaSoft are used for matched KV or matched waterbag beam generation and imported to Impact-Z.**

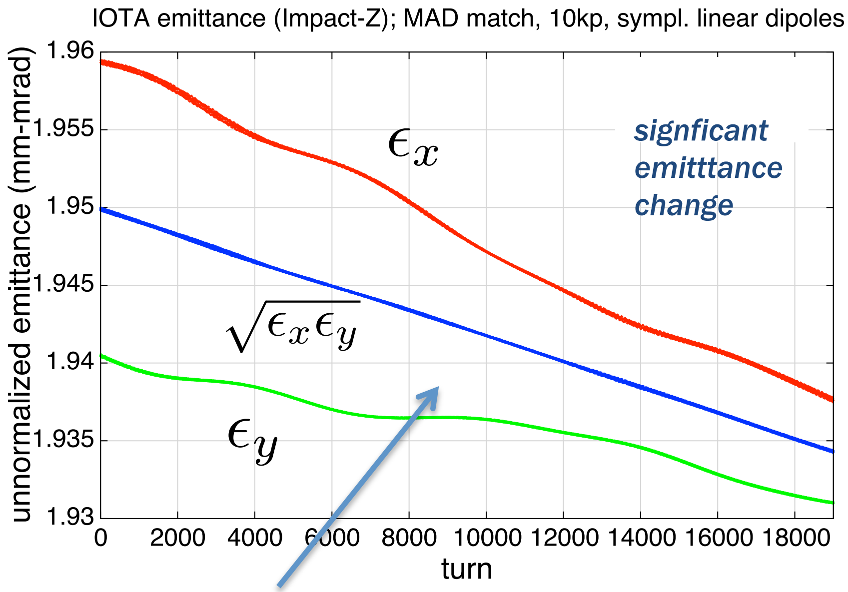
- **Matched beam generation *internal* to Impact-Z will be critical for scaling to large particle numbers, and implementation is in progress.**

[1]S. Webb *et al*, p. 3099, IPAC 2013.

Benchmarks between IMPACT-Z and ML/I resulted in an improvement of IMPACT-Z quad model at low energy.

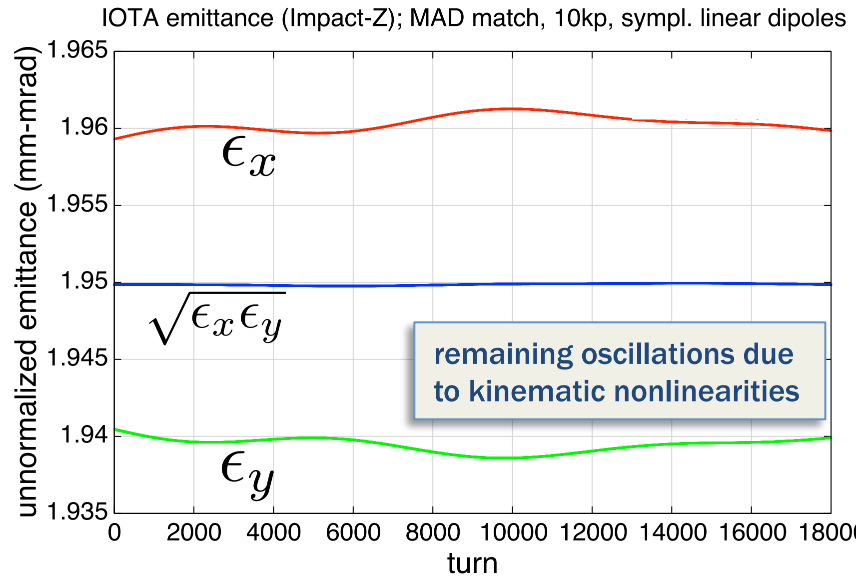
A spurious nonlinear contribution to quadrupole tracking was repaired that is negligible at high energies, but important at the 2.5 MeV *p* energy of IOTA.

Previous quadrupole model



caused by a nonlinear chromatic effect due to energy-dependent normalization of the quadrupole strength *K*

Improved quadrupole model



remaining oscillations due to kinematic nonlinearities